Yttrium alkyl complex with a linked bis(amidinate) ancillary ligand

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"An Yttrium Alkyl Complex with a Linked Bis(amidinate) Ancillary Ligand"

by S. Bambirra, A. Meetsma, B. Hessen,* and J.H. Teuben

Crystal structure determination of $[Me_3SiNC(Ph)N(CH_2)_3NC(Ph)NSiMe_3]Y[CH(SiMe_3)_2](THF)$ (3).

Abstract. "IUPAC-name", $C_{34}H_{61}N_4OSi_4Y$, M = 743.12, monoclinic, $P2_1$, a = 18.763(1), b = 10.205(1), c = 22.391(2) Å, β = 106.383(7) °, V = 4113.3(6) Å^3, Z = 4, D_x = 1.200 g cm^{-3}, λ (MoK$\bar{\alpha}$) = 0.71073 Å, μ = 15.6 cm^{-1}, F(000) = 1584, T = 130 K, $wR(F^2)$ = 0.1128 for 9453 reflections and 818 parameters and $R(F)$ = 0.0487 for 7119 reflections obeying $F_o \geq 4.0\ \sigma(F_o)$ criterion of observability.

The asymmetric unit consists of two molecules of the title compound.

Experimental

X-ray diffraction: Crystal and Molecular Structure.

The crystal, a parallelepiped of approximate size 0.20x 0.25 x 0.50 mm., used for characterization and data collection was glued on top of a glass fiber by using inert-atmosphere handling techniques and was transferred into the cold nitrogen stream of the low temperature unit[1] mounted on an Enraf-Nonius *CAD-4F*[2] diffractometer, interfaced to a *INDY* (*Silicon Graphics*) *UNIX* computer (Mo tube, 50 kV, 40 mA, monochromated Mo-K$\bar{\alpha}$ radiation, $\Delta\omega$ =0.95 + 0.34 tg θ).

Unit cell parameters[3] and orientation matrix were determined from a least-squares treatment of the *SET4*[4] setting angles of 22 reflections in the range 16.77 ° < θ < 21.56 °. The unit cell was identified as monoclinic; reduced cell calculations did not indicate any higher metric lattice symmetry.[5] The $|E|$ distribution statistics[6] were indicative of a non-centrosymmetric space group. The space group, $P2_1$, was determined from considerations of the unit cell parameters, statistical analyses of intensity distributions and where appropriate systematic absences. Examination of the final atomic coordinates in perspective of molecular symmetry and coordinate equivalence suggested a centrosymmetric space group,[7,8] which suggested space group $P2_1/c$, but the systematic extinction's conditions ($h0l$: l=2n+1) was heavily violated.

The intensities of three standard reflections, monitored every three hours of X-ray exposure time, showed no greater fluctuations during data collection than those expected from Poisson statistics. A 360 ° ψ-scan for a reflection close to axial (-204) showed a variation in intensity of less than 7% about the mean value. Intensity data were corrected for Lorentz and polarization effects, scale variation, absorption (*DIFABS*,[9] min. and max. transmission factors 0.456-0.822), and reduced to F_o^2.[10]

The structure was solved by Patterson methods and extension of the model was accomplished by direct methods applied to difference structure factors using the program *DIRDIF*.[11] The positional and

The hydrogen atoms were included in the final refinement riding on their carrier atoms with their positions calculated by using sp^2 or sp^3 hybridization at the C-atom as appropriate with $U_{iso} = c \times U_{equiv}$ of their parent atom, where $c = 1.2$ for the aromatic / non-methyl hydrogen atoms and $c = 1.5$ for the methyl hydrogen atoms and where values U_{equiv} are related to the atoms to which the H atoms are bonded.

Final refinement on F^2 carried out by full-matrix least-squares techniques converged at $wR(F^2) = 0.1128$ for 9453 reflections and $R(F) = 0.0487$ for 7119 reflections with $F_o \geq 4.0\ \sigma(F_o)$ and 818 parameters. The final difference Fourier map was essentially featureless: no significant peaks (0.60(9) e/Å^3) having chemical meaning above the general background were observed. Flack's[12] **x**-refinement give an ambiguous result, probably due to twinning in this respect. Enantiomorph twin refinement resulted in a value of 0.72(2).

The positional and anisotropic displacement parameters for the non-hydrogen atoms and isotropic displacement parameters for hydrogen atoms were refined on F^2 with full-matrix least-squares procedures minimizing the function $Q = \Sigma_h [w(|F_o^2 - kF_c^2|)^2]$, where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, $P = [\max(F_o^2,0) + 2F_c^2] / 3$, F_o and F_c are the observed and calculated structure factor amplitudes, respectively; a and b were refined.

Neutral atom scattering factors and anomalous dispersion corrections were taken from *International Tables for Crystallography.*[13] All calculations performed on the HP9000/735 computer at the University of Groningen with the program packages *SHELXL*[14] (least-square refinements), *PLATON*[15] (calculation of geometric data and the *ORTEP* illustrations) and a locally modified version of the program *PLUTO*[16] (preparation of illustrations).

No missed symmetry (*MISSYM*) or solvent-accessible voids were detected by procedures implemented in *PLATON.*[20,21]

References.

1. Bolhuis, F. van (1971). J. Appl. Cryst. **4**, 263-264.
2. Enraf-Nonius *CAD4-UNIX* Version 5.1, Utrecht modified version October 1994. Enraf-Nonius Delft, Scientific Instruments Division, Delft, The Netherlands.
3. Duisenberg, A. J. M. (1992). J. Appl. Cryst. **25**, 92-96.
4. Boer, J. L. de & Duisenberg, A. J. M. (1984). Acta. Cryst. A**40**, C-410.
5. Spek, A.L. (1988). J. Appl. Cryst. **21**, 578-579
6. Snow, M.R. & Tiekink, E.R.T. (1988). Acta Cryst. B**44**, 676-677.
7. Le Page, Y. (1987). J. Appl. Cryst. **20**, 264-269.
8. Le Page, Y. (1988). J. Appl. Cryst. **21**, 983-984.
9. Walker, N. & Stuart, D. (1983). Acta Cryst. A**39**, 158-166.

10. Spek, A.L. (1993). *HELENA. Program for Reduction of CAD4 Data.* Utrecht Univ. The Netherlands.

11. Beurskens, P.T., Beurskens, G., Bosman, W.P., Gelder, R. de, García-Granda, S., Gould, R.O., Israël, R. & Smits, J.M.M., (1997). The *DIRDIF*-97 program system, Crystallography Laboratory, University of Nijmegen, The Netherlands.

12. Flack, H.D. (1983). Acta. Cryst. A**39**, 876-881.

13. *International Tables for Crystallography* (1992). Vol. C. Edited by A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht. The Netherlands.

14. Sheldrick, G.M. (1997*b*). *SHELXL-97. Program for the Refinement of Crystal Structures.* University of Göttingen, Germany.

15. Spek, A.L. (1998). *PLATON. Program for the Automated Analysis of Molecular Geometry.* Version of March 1998. University of Utrecht, The Netherlands.

16. Meetsma, A. (1996*). PLUTO. Molecular Graphics Program.* University of Groningen, The Netherlands.

17. Hall, S.R, Allen, F.H. & Brown, I.D. (1991). Acta Cryst. A**47**, 655-685.

18. Burnett, M.N. & Johnson, C.K. (1996). *ORTEPIII.* Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.

19. Bondi, A. (1964). J. Phys. Chem. **68**, 441-451.

20. Spek, A.L. (1990). Acta Cryst. A**46**, C-34.

21. Spek, A.L. (1994). Am. Crystallogr. Assoc. Abstr. **22**, 66.

22. *International Tables for Crystallography* (1983). Vol. A. Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel. (Present distributor Kluwer Academic Publishers, Dordrecht).

Fisher, R.X. & Tillmanns, E. (1988). Acta Cryst. C**44**, 775-776.

Table 1.

a. Crystal data and details of the structure determination.

Moiety_ Formula	$C_{34}H_{61}N_4OSi_4Y$
Formula_Weight, g.mol^{-1}	743.12
Crystal system	Monoclinic
Space group, no.[22]	$P2_1$, 4
a, Å	18.763(1)
b, Å	10.205(1)
c, Å	22.391(2)
β, deg	106.383(7)
V, Å^3	4113.3(6)
Formula_*Z*	4
SpaceGroup_*Z*	2
Z' (= Formula_Z / SpaceGroup-*Z*)	2
ρ_{calc}, g.cm^{-3}	1.198
F(000), electrons	1584
μ(Mo K$\bar{\alpha}$), cm^{-1}	15.6
Color, habit	Colorless, parallelepiped
Approx. crystal dimension, mm	0.20 x 0.25 x 0.50

b. Data collection.

Radiation	Mo K$\bar{\alpha}$
Wavelength, Å	0.71073
Monochromator	Graphite
Temperature, K	130
θ range; min. max., deg	1.13, 27.0
ω/2θ scan, deg	$\Delta\omega = 0.95 + 0.34$ tg θ
Index ranges	h: 0→23; k: 0→13; l: -28→27
Crystal-to-receiving-aperture-distance, mm	173
Horizontal-, vertical-aperture, mm	3.2 + tg θ; 4.0
Reference reflections,	-22-2, 2.1
r.m.s. dev. in %	32-1, 2.5
	-224, 2.2
Drift correction	1.000 – 1.013
Min.- max. absorption transmission factor	0.456 - 0.822
X-ray exposure time, h	169.5
Total data	9745
Unique data	9453
Data with criterion: ($F_o \geq 4.0\ \sigma\ (F_o)$)	7119
$R_{int} = \Sigma\ [\lvert F_o^2 - F_o^2\text{(mean)}\rvert] / \Sigma\ [F_o^2]$	0.065
$R_{sig} = \Sigma\ \sigma(F_o^2) / \Sigma\ [F_o^2]$	0.065

c. Refinement.

Number of reflections	9463
Number of refined parameters	818
Final agreement factors:	
$wR(F^2) = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$	0.1128
for $F_o^2 > 0$	
Weighting scheme: *a, b*	0.0322, 8.0825
$w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$	
and $P = [\max(F_o^2,0) + 2F_c^2] / 3$	
$R(F) = \Sigma (\|\|F_o\| - \|F_c\|\|) / \Sigma\|F_o\|$	0.0487
for $F_o > 4.0\ \sigma\ (F_o)$	
Flack's **x** ,Twin ratio	0.72(2)
GooF = S =$[\Sigma [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$	1.020
n = number of reflections	
p = number of parameters refined	
Residual electron density in final	
difference Fourier map, e/Å^3	-0.54, 0.60(9)
Max. (shift/σ) final cycle	< 0.001

Table 2. Final fractional atomic coordinates and equivalent isotropic displacement parameters with s.u.'s in parentheses.

Atoms of the Asymmetric Unit.

Non-Hydrogen parameters

Atom	*x*	*y*	*z*	U_{eq} (Å^2)*
Y(1)	0.76517(4)	1.00833(9)	0.00103(3)	0.02600(19)
Si(1)	0.60137(11)	0.9929(3)	-0.16014(9)	0.0279(6)
Si(2)	0.88586(14)	1.2491(3)	0.13253(11)	0.0433(8)
Si(3)	0.66867(14)	0.8115(3)	0.09383(12)	0.0545(9)
Si(4)	0.62380(15)	1.1059(3)	0.05907(12)	0.0546(10)
O(1)	0.8166(3)	1.1751(8)	-0.0497(3)	0.058(2)
N(1)	0.6869(3)	0.9604(6)	-0.1064(3)	0.0286(17)
N(2)	0.7907(4)	0.8416(8)	-0.0595(3)	0.041(2)
N(3)	0.8604(4)	0.8915(7)	0.0664(3)	0.036(2)
N(4)	0.8576(4)	1.1060(7)	0.0911(3)	0.0305(19)
C(1)	0.5234(4)	0.9364(10)	-0.1310(3)	0.037(3)
C(2)	0.5919(5)	1.1740(9)	-0.1729(4)	0.052(3)
C(3)	0.5907(4)	0.9260(9)	-0.2405(3)	0.039(3)
C(4)	0.7262(4)	0.8505(8)	-0.1045(3)	0.030(3)
C(5)	0.7012(4)	0.7346(8)	-0.1467(3)	0.036(2)
C(6)	0.6514(5)	0.6456(9)	-0.1357(4)	0.047(3)
C(7)	0.6304(6)	0.5386(10)	-0.1753(5)	0.069(4)
C(8)	0.6569(6)	0.5255(12)	-0.2252(5)	0.076(4)
C(9)	0.7065(6)	0.6120(12)	-0.2365(5)	0.069(4)
C(10)	0.7298(5)	0.7172(9)	-0.1981(3)	0.043(3)
C(11)	0.8350(5)	0.7206(11)	-0.0490(5)	0.058(3)
C(12)	0.9060(5)	0.7339(11)	0.0028(4)	0.053(3)
C(13)	0.8943(5)	0.7633(9)	0.0658(4)	0.040(3)
C(14)	0.8935(4)	0.9893(8)	0.1008(3)	0.027(2)
C(15)	0.9683(4)	0.9732(8)	0.1473(3)	0.032(2)
C(16)	1.0328(4)	0.9997(11)	0.1311(4)	0.046(3)
C(17)	1.1021(5)	0.9869(10)	0.1745(4)	0.056(3)
C(18)	1.1063(5)	0.947(1)	0.2333(4)	0.057(3)
C(19)	1.0430(6)	0.9196(10)	0.2495(4)	0.055(3)
C(20)	0.9737(5)	0.9334(9)	0.2078(3)	0.043(3)
C(21)	0.9773(6)	1.3117(11)	0.1271(6)	0.078(4)
C(22)	0.8909(6)	1.2323(11)	0.2161(4)	0.066(4)
C(23)	0.8178(5)	1.3795(10)	0.0971(4)	0.066(4)
C(24)	0.6626(4)	0.9502(9)	0.0407(3)	0.034(3)
C(25)	0.6816(6)	0.6552(11)	0.0537(5)	0.074(4)
C(26)	0.7479(5)	0.8272(14)	0.1679(4)	0.088(5)
C(27)	0.5831(5)	0.7864(14)	0.1209(4)	0.074(4)
C(28)	0.6397(6)	1.2328(11)	0.0040(5)	0.073(4)
C(29)	0.6693(6)	1.1608(13)	0.1387(5)	0.087(5)
C(30)	0.5209(5)	1.1047(13)	0.0485(5)	0.084(5)
C(31)	0.7842(7)	1.2506(16)	-0.1013(6)	0.107(6)
C(32)	0.8087(10)	1.179(2)	-0.1508(5)	0.145(9)
C(33)	0.8872(10)	1.1358(18)	-0.1158(7)	0.126(8)
C(34)	0.8908(6)	1.1561(14)	-0.0504(5)	0.073(5)

Residue: 2.

Y(2)	0.24247(4)	0.55792(8)	0.50644(3)	0.0251(2)

Si(6)	0.40870(12)	0.5998(2)	0.66613(9)	0.0282(6)
Si(7)	0.38587(13)	0.4317(3)	0.45853(10)	0.0352(7)
Si(8)	0.33383(13)	0.7047(3)	0.3947(1)	0.0361(7)
O(2)	0.1892(3)	0.4093(7)	0.5651(3)	0.052(2)
N(5)	0.1502(4)	0.4453(7)	0.4218(3)	0.035(2)
N(6)	0.1459(4)	0.6632(7)	0.4364(3)	0.0296(19)
N(7)	0.2195(4)	0.7371(8)	0.5593(3)	0.043(2)
N(8)	0.3223(3)	0.6278(6)	0.6118(3)	0.0262(17)
C(35)	0.1909(5)	0.1715(9)	0.4344(4)	0.058(3)
C(36)	0.1257(5)	0.2915(10)	0.3048(4)	0.062(3)
C(37)	0.0305(5)	0.2355(11)	0.3892(5)	0.063(4)
C(38)	0.1138(4)	0.5569(9)	0.4073(3)	0.032(2)
C(39)	0.0379(4)	0.5670(8)	0.3602(3)	0.032(2)
C(40)	0.0313(5)	0.5922(8)	0.2988(3)	0.040(3)
C(41)	-0.0377(6)	0.6011(10)	0.2551(4)	0.063(3)
C(42)	-0.1006(5)	0.5878(9)	0.2738(5)	0.060(3)
C(43)	-0.0954(5)	0.5647(11)	0.3353(5)	0.055(3)
C(44)	-0.0261(5)	0.5542(12)	0.3790(4)	0.050(3)
C(45)	0.1098(4)	0.7907(8)	0.4325(3)	0.034(2)
C(46)	0.1022(5)	0.8337(10)	0.4951(4)	0.046(3)
C(47)	0.1751(6)	0.8568(11)	0.5453(4)	0.062(3)
C(48)	0.2830(4)	0.7372(8)	0.6044(3)	0.031(2)
C(49)	0.3069(4)	0.8587(9)	0.6428(3)	0.033(2)
C(50)	0.2829(4)	0.8836(9)	0.6943(3)	0.039(3)
C(51)	0.3069(5)	0.9957(10)	0.7306(4)	0.049(3)
C(52)	0.3548(5)	1.0815(8)	0.7139(4)	0.051(3)
C(53)	0.3787(5)	1.056(1)	0.6615(4)	0.049(3)
C(54)	0.3547(5)	0.9453(9)	0.6260(4)	0.042(3)
C(55)	0.4313(4)	0.7013(9)	0.7377(3)	0.044(3)
C(56)	0.4123(5)	0.4293(8)	0.6955(4)	0.046(3)
C(57)	0.4848(4)	0.6245(11)	0.6302(4)	0.047(3)
C(58)	0.3442(4)	0.5936(9)	0.4606(4)	0.035(3)
C(59)	0.3684(5)	0.3249(10)	0.5223(4)	0.048(3)
C(60)	0.4888(4)	0.4331(11)	0.4727(4)	0.049(3)
C(61)	0.3461(5)	0.3417(9)	0.3835(4)	0.049(3)
C(62)	0.4197(5)	0.7204(10)	0.3669(3)	0.045(3)
C(63)	0.2574(5)	0.6548(10)	0.3247(3)	0.054(3)
C(64)	0.3118(5)	0.8750(9)	0.4168(5)	0.057(3)
C(65)	0.1122(5)	0.4230(18)	0.5608(5)	0.094(6)
C(66)	0.1082(8)	0.4371(19)	0.6260(6)	0.104(7)
C(67)	0.1825(10)	0.413(2)	0.6642(5)	0.132(8)
C(68)	0.2208(6)	0.3535(16)	0.6237(6)	0.108(6)

Hydrogen parameters

Atom	*x*	*y*	*z*	*Ueq (Å2)**
H(1)	0.52610(-)	0.84104(-)	-0.12558(-)	0.05551(-)
H(1')	0.47612(-)	0.95994(-)	-0.16100(-)	0.05551(-)
H(1'')	0.52676(-)	0.97833(-)	-0.09089(-)	0.05551(-)
H(2)	0.60129(-)	1.21861(-)	-0.13268(-)	0.07843(-)
H(2')	0.54156(-)	1.19441(-)	-0.19857(-)	0.07843(-)
H(2'')	0.62802(-)	1.20392(-)	-0.19420(-)	0.07843(-)
H(3)	0.63536(-)	0.94633(-)	-0.25327(-)	0.05879(-)
H(3')	0.54732(-)	0.96599(-)	-0.26983(-)	0.05879(-)

H(6)	0.63144(-)	0.65707(-)	-0.10150(-)	0.05647(-)
H(7)	0.59749(-)	0.47464(-)	-0.16725(-)	0.08215(-)
H(8)	0.64049(-)	0.45418(-)	-0.25288(-)	0.09148(-)
H(9)	0.72506(-)	0.59943(-)	-0.27144(-)	0.08336(-)
H(10)	0.76468(-)	0.77756(-)	-0.20595(-)	0.05120(-)
H(11)	0.84714(-)	0.69672(-)	-0.08789(-)	0.07041(-)
H(11')	0.80495(-)	0.64868(-)	-0.03889(-)	0.07041(-)
H(12)	0.93614(-)	0.80499(-)	-0.00785(-)	0.06272(-)
H(12')	0.93461(-)	0.65147(-)	0.00587(-)	0.06272(-)
H(13)	0.86204(-)	0.69513(-)	0.07597(-)	0.04814(-)
H(13')	0.94280(-)	0.76070(-)	0.09819(-)	0.04814(-)
H(16)	1.02973(-)	1.02687(-)	0.08983(-)	0.05457(-)
H(17)	1.14612(-)	1.00587(-)	0.16316(-)	0.06719(-)
H(18)	1.15338(-)	0.93824(-)	0.26315(-)	0.06873(-)
H(19)	1.04680(-)	0.89025(-)	0.29060(-)	0.06579(-)
H(20)	0.93019(-)	0.91591(-)	0.22013(-)	0.05139(-)
H(21)	1.01728(-)	1.25746(-)	0.15306(-)	0.11637(-)
H(21')	0.98383(-)	1.40256(-)	0.14178(-)	0.11637(-)
H(21")	0.97872(-)	1.30781(-)	0.08378(-)	0.11637(-)
H(22)	0.84836(-)	1.18109(-)	0.22022(-)	0.09882(-)
H(22')	0.88995(-)	1.31938(-)	0.23428(-)	0.09882(-)
H(22")	0.93710(-)	1.18745(-)	0.23795(-)	0.09882(-)
H(23)	0.80941(-)	1.37978(-)	0.05184(-)	0.09930(-)
H(23')	0.83730(-)	1.46491(-)	0.11411(-)	0.09930(-)
H(23")	0.77071(-)	1.36258(-)	0.10655(-)	0.09930(-)
H(24)	0.62403(-)	0.92031(-)	0.00245(-)	0.04043(-)
H(25)	0.64275(-)	0.64806(-)	0.01403(-)	0.11098(-)
H(25')	0.67835(-)	0.58036(-)	0.08021(-)	0.11098(-)
H(25")	0.73045(-)	0.65579(-)	0.04592(-)	0.11098(-)
H(26)	0.79539(-)	0.82099(-)	0.15792(-)	0.13179(-)
H(26')	0.74458(-)	0.75667(-)	0.19671(-)	0.13179(-)
H(26")	0.74471(-)	0.91216(-)	0.18744(-)	0.13179(-)
H(27)	0.58131(-)	0.85350(-)	0.15177(-)	0.11101(-)
H(27')	0.58489(-)	0.69935(-)	0.13980(-)	0.11101(-)
H(27")	0.53873(-)	0.79323(-)	0.08530(-)	0.11101(-)
H(28)	0.69189(-)	1.23076(-)	0.00388(-)	0.10892(-)
H(28')	0.62785(-)	1.31960(-)	0.01735(-)	0.10892(-)
H(28")	0.60779(-)	1.21460(-)	-0.03797(-)	0.10892(-)
H(29)	0.66194(-)	1.09506(-)	0.16832(-)	0.13029(-)
H(29')	0.64763(-)	1.24436(-)	0.14635(-)	0.13029(-)
H(29")	0.72256(-)	1.17232(-)	0.14401(-)	0.13029(-)
H(30)	0.49510(-)	1.07648(-)	0.00605(-)	0.12625(-)
H(30')	0.50440(-)	1.19302(-)	0.05548(-)	0.12625(-)
H(30")	0.50947(-)	1.04388(-)	0.07839(-)	0.12625(-)
H(31)	0.80309(-)	1.34170(-)	-0.09613(-)	0.12885(-)
H(31')	0.72936(-)	1.25168(-)	-0.11048(-)	0.12885(-)
H(32)	0.80888(-)	1.23781(-)	-0.18594(-)	0.17460(-)
H(32')	0.77624(-)	1.10287(-)	-0.16674(-)	0.17460(-)
H(33)	0.89523(-)	1.04247(-)	-0.12412(-)	0.15120(-)
H(33')	0.92479(-)	1.18971(-)	-0.12781(-)	0.15120(-)
H(34)	0.91250(-)	1.07858(-)	-0.02521(-)	0.08735(-)
H(34')	0.92136(-)	1.23387(-)	-0.03357(-)	0.08735(-)

Residue: 2.

H(35")	0.19136(-)	0.17760(-)	0.47815(-)	0.08695(-)
H(36)	0.08087(-)	0.33413(-)	0.27866(-)	0.09325(-)
H(36')	0.12734(-)	0.20048(-)	0.29125(-)	0.09325(-)
H(36")	0.16973(-)	0.33831(-)	0.30082(-)	0.09325(-)
H(37)	0.02975(-)	0.22465(-)	0.43251(-)	0.09392(-)
H(37')	0.01994(-)	0.15124(-)	0.36753(-)	0.09392(-)
H(37")	-0.00723(-)	0.29967(-)	0.36849(-)	0.09392(-)
H(40)	0.07492(-)	0.60373(-)	0.28579(-)	0.04830(-)
H(41)	-0.04113(-)	0.61645(-)	0.21257(-)	0.07528(-)
H(42)	-0.14804(-)	0.59439(-)	0.24416(-)	0.07185(-)
H(43)	-0.13933(-)	0.55586(-)	0.34814(-)	0.06564(-)
H(44)	-0.02267(-)	0.53840(-)	0.42152(-)	0.05961(-)
H(45)	0.06000(-)	0.78613(-)	0.40221(-)	0.04131(-)
H(45')	0.13937(-)	0.85654(-)	0.41733(-)	0.04131(-)
H(46)	0.07358(-)	0.76611(-)	0.51019(-)	0.05483(-)
H(46')	0.07286(-)	0.91575(-)	0.48923(-)	0.05483(-)
H(47)	0.20388(-)	0.92546(-)	0.53109(-)	0.07489(-)
H(47')	0.16439(-)	0.88864(-)	0.58362(-)	0.07489(-)
H(50)	0.24981(-)	0.82420(-)	0.70536(-)	0.04677(-)
H(51)	0.29031(-)	1.01241(-)	0.76630(-)	0.05921(-)
H(52)	0.37152(-)	1.15782(-)	0.73802(-)	0.06082(-)
H(53)	0.41170(-)	1.11516(-)	0.65003(-)	0.05850(-)
H(54)	0.37102(-)	0.92856(-)	0.59027(-)	0.04978(-)
H(55)	0.43736(-)	0.79289(-)	0.72687(-)	0.06581(-)
H(55')	0.47762(-)	0.66987(-)	0.76667(-)	0.06581(-)
H(55")	0.39097(-)	0.69484(-)	0.75738(-)	0.06581(-)
H(56)	0.37738(-)	0.41957(-)	0.72044(-)	0.06807(-)
H(56')	0.46277(-)	0.40967(-)	0.72124(-)	0.06807(-)
H(56")	0.39881(-)	0.36849(-)	0.66016(-)	0.06807(-)
H(57)	0.47830(-)	0.56480(-)	0.59479(-)	0.06937(-)
H(57')	0.53245(-)	0.60668(-)	0.66096(-)	0.06937(-)
H(57")	0.48404(-)	0.71529(-)	0.61571(-)	0.06937(-)
H(58)	0.38220(-)	0.63900(-)	0.49479(-)	0.04172(-)
H(59)	0.39267(-)	0.36382(-)	0.56295(-)	0.07199(-)
H(59')	0.38877(-)	0.23719(-)	0.51998(-)	0.07199(-)
H(59")	0.31487(-)	0.31850(-)	0.51682(-)	0.07199(-)
H(60)	0.50103(-)	0.47283(-)	0.43701(-)	0.07364(-)
H(60')	0.50766(-)	0.34307(-)	0.47835(-)	0.07364(-)
H(60")	0.51175(-)	0.48420(-)	0.51030(-)	0.07364(-)
H(61)	0.29214(-)	0.35412(-)	0.36974(-)	0.07382(-)
H(61')	0.35738(-)	0.24807(-)	0.38983(-)	0.07382(-)
H(61")	0.36803(-)	0.37579(-)	0.35178(-)	0.07382(-)
H(62)	0.46161(-)	0.74931(-)	0.40144(-)	0.06793(-)
H(62')	0.41070(-)	0.78484(-)	0.33310(-)	0.06793(-)
H(62")	0.43138(-)	0.63530(-)	0.35167(-)	0.06793(-)
H(63)	0.26722(-)	0.56639(-)	0.31187(-)	0.08141(-)
H(63')	0.25503(-)	0.71642(-)	0.29065(-)	0.08141(-)
H(63")	0.21000(-)	0.65546(-)	0.33501(-)	0.08141(-)
H(64)	0.26861(-)	0.87192(-)	0.43309(-)	0.08517(-)
H(64')	0.30085(-)	0.93166(-)	0.37993(-)	0.08517(-)
H(64")	0.35464(-)	0.91010(-)	0.44869(-)	0.08517(-)
H(65)	0.08418(-)	0.34476(-)	0.54094(-)	0.11280(-)
H(65')	0.09124(-)	0.50126(-)	0.53594(-)	0.11280(-)
H(66)	0.09176(-)	0.52637(-)	0.63321(-)	0.12431(-)
H(66')	0.07314(-)	0.37262(-)	0.63490(-)	0.12431(-)

H(68)	0.27467(-)	0.37264(-)	0.63831(-)	0.13003(-)
H(68')	0.21367(-)	0.25735(-)	0.62215(-)	0.13003(-)

*) $U_{eq} = 1/3 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j$ Error! Reference source not found.

Anisotropic (displacement) parameters (Å^2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Y(1)	0.0248(3)	0.0259(4)	0.0275(3)	-0.0025(3)	0.0077(3)	0.0002(3)
Si(1)	0.0277(10)	0.0302(11)	0.0256(9)	0.0019(9)	0.0074(8)	0.0005(10)
Si(2)	0.0466(14)	0.0321(13)	0.0470(13)	-0.0109(10)	0.0063(11)	-0.0027(11)
Si(3)	0.0343(13)	0.084(2)	0.0434(13)	0.0198(14)	0.0082(10)	-0.0094(14)
Si(4)	0.0412(14)	0.074(2)	0.0531(15)	-0.0189(14)	0.0206(12)	0.0036(13)
O(1)	0.031(3)	0.068(5)	0.069(4)	0.030(4)	0.006(3)	-0.013(3)
N(1)	0.028(3)	0.026(3)	0.036(3)	0.002(3)	0.016(3)	0.006(3)
N(2)	0.035(4)	0.042(4)	0.043(4)	-0.015(3)	0.007(3)	0.016(3)
N(3)	0.032(4)	0.035(4)	0.039(4)	-0.004(3)	0.006(3)	0.005(3)
N(4)	0.035(4)	0.023(3)	0.033(3)	-0.005(3)	0.009(3)	-0.004(3)
C(1)	0.034(4)	0.046(5)	0.031(4)	-0.002(4)	0.008(3)	-0.001(4)
C(2)	0.049(5)	0.036(5)	0.061(6)	0.005(4)	-0.002(4)	-0.001(4)
C(3)	0.039(4)	0.046(5)	0.032(4)	0.008(4)	0.008(3)	0.000(4)
C(4)	0.028(4)	0.037(5)	0.028(4)	-0.010(3)	0.014(3)	-0.004(3)
C(5)	0.034(4)	0.032(4)	0.033(4)	-0.006(3)	-0.005(3)	0.009(4)
C(6)	0.044(5)	0.038(5)	0.054(5)	-0.007(4)	0.005(4)	0.004(4)
C(7)	0.064(6)	0.028(6)	0.096(8)	0.000(5)	-0.006(6)	-0.008(5)
C(8)	0.074(7)	0.062(9)	0.064(7)	-0.037(6)	-0.027(6)	0.029(6)
C(9)	0.067(7)	0.076(8)	0.051(6)	-0.032(6)	-0.006(5)	0.025(6)
C(10)	0.043(5)	0.048(5)	0.034(4)	-0.014(4)	0.005(3)	0.019(4)
C(11)	0.044(5)	0.058(7)	0.063(6)	-0.026(5)	-0.002(4)	0.024(5)
C(12)	0.047(5)	0.055(6)	0.053(5)	-0.006(5)	0.009(4)	0.019(5)
C(13)	0.035(5)	0.035(5)	0.044(5)	-0.006(4)	0.002(4)	-0.002(4)
C(14)	0.028(4)	0.031(4)	0.023(3)	-0.002(3)	0.007(3)	0.001(3)
C(15)	0.030(4)	0.023(4)	0.039(4)	-0.003(3)	0.003(3)	-0.003(3)
C(16)	0.039(4)	0.039(5)	0.057(5)	0.006(5)	0.011(4)	0.001(5)
C(17)	0.040(5)	0.044(6)	0.072(6)	-0.003(5)	-0.004(4)	-0.001(5)
C(18)	0.048(6)	0.040(5)	0.063(6)	-0.005(5)	-0.019(5)	0.002(4)
C(19)	0.064(6)	0.048(6)	0.041(5)	0.009(4)	-0.004(4)	-0.015(5)
C(20)	0.050(5)	0.041(5)	0.034(4)	0.009(4)	0.007(4)	-0.010(4)
C(21)	0.061(7)	0.052(7)	0.120(9)	-0.041(7)	0.024(6)	-0.015(6)
C(22)	0.091(8)	0.058(7)	0.051(5)	-0.024(5)	0.023(5)	-0.017(6)
C(23)	0.074(7)	0.039(5)	0.075(7)	-0.017(5)	0.003(5)	0.008(5)
C(24)	0.025(4)	0.050(5)	0.027(4)	-0.007(4)	0.009(3)	-0.002(4)
C(25)	0.052(6)	0.061(7)	0.103(9)	0.019(6)	0.014(6)	-0.004(5)
C(26)	0.064(7)	0.146(13)	0.041(5)	0.044(7)	-0.004(5)	-0.021(8)
C(27)	0.061(6)	0.124(11)	0.039(5)	0.009(6)	0.017(4)	-0.022(7)
C(28)	0.076(7)	0.059(7)	0.076(7)	-0.007(6)	0.009(6)	0.011(6)
C(29)	0.092(9)	0.096(10)	0.091(8)	-0.037(7)	0.056(7)	-0.019(8)
C(30)	0.057(6)	0.096(10)	0.108(9)	-0.031(8)	0.036(6)	0.014(6)
C(31)	0.085(9)	0.120(12)	0.094(9)	0.069(9)	-0.013(7)	-0.042(8)
C(32)	0.161(16)	0.22(2)	0.034(6)	0.001(9)	-0.004(8)	-0.128(16)
C(33)	0.173(17)	0.101(12)	0.143(14)	-0.033(11)	0.109(13)	-0.050(13)
C(34)	0.058(7)	0.083(9)	0.084(8)	0.002(7)	0.029(6)	-0.022(7)

Residue: 2.

Y(2)	0.0268(4)	0.0239(4)	0.0250(3)	-0.0003(3)	0.0082(3)	0.0010(3)
Si(5)	0.0421(13)	0.0297(12)	0.0486(13)	-0.0131(10)	0.0109(10)	-0.0065(10)
Si(6)	0.0301(11)	0.0279(11)	0.0257(10)	0.0015(8)	0.0062(8)	-0.0023(9)
Si(7)	0.0338(12)	0.0434(13)	0.0312(11)	0.0001(10)	0.0135(9)	0.0091(10)
Si(8)	0.0345(12)	0.0421(14)	0.0337(11)	0.0061(10)	0.0128(9)	0.0039(10)
O(2)	0.033(3)	0.063(4)	0.059(4)	0.027(3)	0.010(3)	-0.005(3)
N(5)	0.035(4)	0.028(4)	0.040(4)	-0.003(3)	0.006(3)	0.005(3)
N(6)	0.032(4)	0.023(3)	0.028(3)	-0.006(3)	-0.001(3)	0.000(3)
N(7)	0.047(4)	0.045(5)	0.029(3)	-0.010(3)	-0.003(3)	0.021(4)
N(8)	0.033(3)	0.022(3)	0.023(3)	-0.002(2)	0.007(2)	-0.003(3)
C(35)	0.071(6)	0.030(5)	0.067(6)	-0.006(4)	0.011(5)	-0.003(5)
C(36)	0.067(6)	0.056(6)	0.057(6)	-0.026(5)	0.007(5)	-0.004(5)
C(37)	0.063(7)	0.049(6)	0.085(7)	-0.016(6)	0.035(6)	-0.013(5)
C(38)	0.031(4)	0.035(4)	0.031(4)	-0.001(4)	0.012(3)	-0.006(4)
C(39)	0.031(4)	0.023(4)	0.040(4)	0.000(4)	0.005(3)	-0.002(4)
C(40)	0.042(5)	0.039(5)	0.031(4)	0.004(3)	-0.003(3)	-0.002(4)
C(41)	0.072(7)	0.053(6)	0.045(5)	0.002(4)	-0.014(5)	-0.007(5)
C(42)	0.044(5)	0.038(6)	0.078(7)	-0.004(5)	-0.015(5)	-0.001(4)
C(43)	0.032(4)	0.049(6)	0.082(7)	0.000(6)	0.015(4)	-0.002(5)
C(44)	0.038(4)	0.058(6)	0.052(5)	0.005(5)	0.010(4)	-0.001(5)
C(45)	0.032(4)	0.024(4)	0.040(4)	0.002(3)	-0.002(3)	0.010(4)
C(46)	0.043(5)	0.046(6)	0.045(5)	-0.012(4)	0.008(4)	0.022(4)
C(47)	0.061(6)	0.061(7)	0.046(5)	-0.029(5)	-0.015(4)	0.035(5)
C(48)	0.041(4)	0.029(4)	0.023(3)	-0.001(3)	0.008(3)	0.004(4)
C(49)	0.036(4)	0.038(5)	0.022(3)	-0.003(3)	0.005(3)	0.008(4)
C(50)	0.041(4)	0.044(5)	0.032(4)	-0.001(4)	0.011(3)	0.000(4)
C(51)	0.049(5)	0.054(6)	0.042(4)	-0.022(5)	0.008(4)	0.019(5)
C(52)	0.064(6)	0.022(5)	0.055(5)	-0.005(4)	-0.002(4)	0.005(4)
C(53)	0.050(5)	0.034(4)	0.060(5)	0.007(5)	0.010(4)	-0.005(5)
C(54)	0.049(5)	0.037(5)	0.038(4)	0.005(4)	0.010(4)	0.002(4)
C(55)	0.045(5)	0.049(5)	0.035(4)	0.003(4)	0.007(3)	0.002(4)
C(56)	0.053(5)	0.035(5)	0.041(5)	0.004(4)	0.001(4)	-0.006(4)
C(57)	0.032(4)	0.067(7)	0.038(4)	0.002(5)	0.005(4)	0.002(5)
C(58)	0.032(4)	0.034(5)	0.040(4)	-0.010(3)	0.014(3)	-0.001(4)
C(59)	0.056(6)	0.045(5)	0.043(5)	0.004(4)	0.014(4)	0.002(4)
C(60)	0.040(5)	0.065(6)	0.043(4)	-0.002(4)	0.012(4)	0.015(5)
C(61)	0.052(5)	0.054(6)	0.044(5)	-0.002(4)	0.017(4)	0.003(4)
C(62)	0.050(5)	0.057(6)	0.032(4)	0.000(4)	0.017(4)	-0.003(4)
C(63)	0.052(5)	0.076(7)	0.029(4)	0.011(4)	0.004(4)	0.001(5)
C(64)	0.054(6)	0.041(5)	0.079(7)	0.012(5)	0.024(5)	0.013(4)
C(65)	0.032(5)	0.181(15)	0.068(7)	0.053(9)	0.013(5)	-0.009(8)
C(66)	0.109(11)	0.133(13)	0.099(10)	0.025(10)	0.078(9)	0.037(10)
C(67)	0.157(14)	0.196(19)	0.037(6)	0.002(9)	0.018(8)	-0.095(14)
C(68)	0.044(6)	0.161(15)	0.104(9)	0.103(11)	-0.006(6)	-0.010(8)

Thermal vibration amplitudes ($Å^2$)

$$F(\mathbf{h}) = F_o(\mathbf{h}) \exp\left(-2\pi^2 \sum_{i=1}^{3}\sum_{j=1}^{3} h_i h_i a_i^* a_j^* U_{ij}\right)$$

or

$$F(\mathbf{h}) = F_o(\mathbf{h}) \exp\left(-8\pi^2 U_{iso} (\sin(\theta)/\lambda)^2\right)$$

Table 3. Selected data on the geometry.

Standard deviations in the last decimal place are given in parentheses.

Residue: 1.
Interatomic Distances (Å)

Y(1)	-O(1)	2.395(7)	N(1)	-C(4)	1.336(10)
Y(1)	-N(1)	2.488(6)	N(2)	-C(4)	1.342(10)
Y(1)	-N(2)	2.308(8)	N(2)	-C(11)	1.470(14)
Y(1)	-N(3)	2.298(7)	N(3)	-C(13)	1.456(12)
Y(1)	-N(4)	2.469(7)	N(3)	-C(14)	1.306(10)
Y(1)	-C(4)	2.782(7)	N(4)	-C(14)	1.355(11)
Y(1)	-C(14)	2.791(7)	C(4)	-C(5)	1.504(11)
Y(1)	-C(24)	2.410(8)	C(5)	-C(6)	1.374(12)
Si(1)	-N(1)	1.745(7)	C(5)	-C(10)	1.412(10)
Si(1)	-C(1)	1.854(8)	C(6)	-C(7)	1.392(14)
Si(1)	-C(2)	1.871(10)	C(7)	-C(8)	1.352(16)
Si(1)	-C(3)	1.882(7)	C(8)	-C(9)	1.357(17)
Si(2)	-N(4)	1.731(8)	C(9)	-C(10)	1.368(14)
Si(2)	-C(21)	1.867(12)	C(11)	-C(12)	1.506(14)
Si(2)	-C(22)	1.855(9)	C(12)	-C(13)	1.517(13)
Si(2)	-C(23)	1.86(1)	C(14)	-C(15)	1.502(10)
Si(3)	-C(24)	1.832(9)	C(15)	-C(16)	1.385(11)
Si(3)	-C(25)	1.880(12)	C(15)	-C(20)	1.39(1)
Si(3)	-C(26)	1.896(9)	C(16)	-C(17)	1.393(12)
Si(3)	-C(27)	1.887(10)	C(17)	-C(18)	1.359(12)
Si(4)	-C(24)	1.842(9)	C(18)	-C(19)	1.365(15)
Si(4)	-C(28)	1.869(11)	C(19)	-C(20)	1.377(13)
Si(4)	-C(29)	1.834(11)	C(31)	-C(32)	1.50(2)
Si(4)	-C(30)	1.878(10)	C(32)	-C(33)	1.53(3)
O(1)	-C(31)	1.379(16)	C(33)	-C(34)	1.462(19)
O(1)	-C(34)	1.410(13)			

Bond Angles (deg.)

O(1)	-Y(1)	-N(1)	83.6(2)	C(28)	-Si(4)	-C(29)	108.2(5)
O(1)	-Y(1)	-N(2)	93.9(3)	C(28)	-Si(4)	-C(30)	105.7(5)
O(1)	-Y(1)	-N(3)	109.0(2)	C(29)	-Si(4)	-C(30)	107.7(5)
O(1)	-Y(1)	-N(4)	79.4(2)	Y(1)	-O(1)	-C(31)	130.8(7)
O(1)	-Y(1)	-C(4)	93.0(2)	Y(1)	-O(1)	-C(34)	116.0(7)
O(1)	-Y(1)	-C(14)	93.3(2)	C(31)	-O(1)	-C(34)	105.7(9)
O(1)	-Y(1)	-C(24)	145.1(3)	Y(1)	-N(1)	-Si(1)	143.8(3)
N(1)	-Y(1)	-N(2)	56.7(2)	Y(1)	-N(1)	-C(4)	88.0(4)
N(1)	-Y(1)	-N(3)	130.9(2)	Si(1)	-N(1)	-C(4)	125.0(5)
N(1)	-Y(1)	-N(4)	163.0(2)	Y(1)	-N(2)	-C(4)	95.6(5)
N(1)	-Y(1)	-C(4)	28.7(2)	Y(1)	-N(2)	-C(11)	136.6(6)
N(1)	-Y(1)	-C(14)	154.3(2)	C(4)	-N(2)	-C(11)	121.8(8)
N(1)	-Y(1)	-C(24)	89.6(2)	Y(1)	-N(3)	-C(13)	136.3(5)
N(2)	-Y(1)	-N(3)	74.9(2)	Y(1)	-N(3)	-C(14)	97.7(5)
N(2)	-Y(1)	-N(4)	124.3(3)	C(13)	-N(3)	-C(14)	123.8(7)
N(2)	-Y(1)	-C(4)	28.7(2)	Y(1)	-N(4)	-Si(2)	144.8(4)
N(2)	-Y(1)	-C(14)	98.3(2)	Y(1)	-N(4)	-C(14)	88.8(4)
N(2)	-Y(1)	-C(24)	110.8(3)	Si(2)	-N(4)	-C(14)	126.3(6)
N(3)	-Y(1)	-N(4)	56.5(2)	Y(1)	-C(4)	-N(1)	63.4(4)

N(3)	-Y(1)	-C(24)	101.3(3)
N(4)	-Y(1)	-C(4)	152.1(2)
N(4)	-Y(1)	-C(14)	29.0(2)
N(4)	-Y(1)	-C(24)	104.4(2)
C(4)	-Y(1)	-C(14)	126.9(2)
C(4)	-Y(1)	-C(24)	97.2(2)
C(14)	-Y(1)	-C(24)	106.6(2)
N(1)	-Si(1)	-C(1)	111.2(3)
N(1)	-Si(1)	-C(2)	108.8(4)
N(1)	-Si(1)	-C(3)	114.8(3)
C(1)	-Si(1)	-C(2)	108.1(4)
C(1)	-Si(1)	-C(3)	110.0(4)
C(2)	-Si(1)	-C(3)	103.4(4)
N(4)	-Si(2)	-C(21)	113.7(5)
N(4)	-Si(2)	-C(22)	112.5(4)
N(4)	-Si(2)	-C(23)	107.8(4)
C(21)	-Si(2)	-C(22)	108.1(5)
C(21)	-Si(2)	-C(23)	105.1(5)
C(22)	-Si(2)	-C(23)	109.3(5)
C(24)	-Si(3)	-C(25)	109.8(4)
C(24)	-Si(3)	-C(26)	113.1(5)
C(24)	-Si(3)	-C(27)	114.3(5)
C(25)	-Si(3)	-C(26)	108.3(5)
C(25)	-Si(3)	-C(27)	105.9(6)
C(26)	-Si(3)	-C(27)	105.0(4)
C(24)	-Si(4)	-C(28)	107.7(4)
C(24)	-Si(4)	-C(29)	112.1(5)
C(24)	-Si(4)	-C(30)	115.0(5)
Y(1)	-C(24)	-Si(3)	121.3(4)
Y(1)	-C(24)	-Si(4)	106.1(4)
Si(3)	-C(24)	-Si(4)	118.5(4)
O(1)	-C(31)	-C(32)	101.1(12)
N(1)	-C(4)	-N(2)	117.0(7)
N(1)	-C(4)	-C(5)	124.6(6)
N(2)	-C(4)	-C(5)	118.3(7)
C(4)	-C(5)	-C(6)	121.0(7)
C(4)	-C(5)	-C(10)	119.2(7)
C(6)	-C(5)	-C(10)	119.8(8)
C(5)	-C(6)	-C(7)	119.3(8)
C(6)	-C(7)	-C(8)	120.(1)
C(7)	-C(8)	-C(9)	121.4(11)
C(8)	-C(9)	-C(10)	120.5(10)
C(5)	-C(10)	-C(9)	118.9(9)
N(2)	-C(11)	-C(12)	112.6(9)
C(11)	-C(12)	-C(13)	113.9(8)
N(3)	-C(13)	-C(12)	111.4(7)
Y(1)	-C(14)	-N(3)	54.7(4)
Y(1)	-C(14)	-N(4)	62.2(4)
Y(1)	-C(14)	-C(15)	171.4(5)
N(3)	-C(14)	-N(4)	116.4(7)
N(3)	-C(14)	-C(15)	121.4(7)
N(4)	-C(14)	-C(15)	122.2(7)
C(14)	-C(15)	-C(16)	120.8(6)
C(14)	-C(15)	-C(20)	120.3(7)
C(16)	-C(15)	-C(20)	118.9(7)
C(15)	-C(16)	-C(17)	120.8(8)
C(16)	-C(17)	-C(18)	119.5(9)
C(17)	-C(18)	-C(19)	120.1(9)
C(18)	-C(19)	-C(20)	121.6(8)
C(15)	-C(20)	-C(19)	119.1(8)
C(31)	-C(32)	-C(33)	102.3(11)
C(32)	-C(33)	-C(34)	103.8(13)
O(1)	-C(34)	-C(33)	105.3(11)

Residue: 2.
Interatomic Distances (Å)

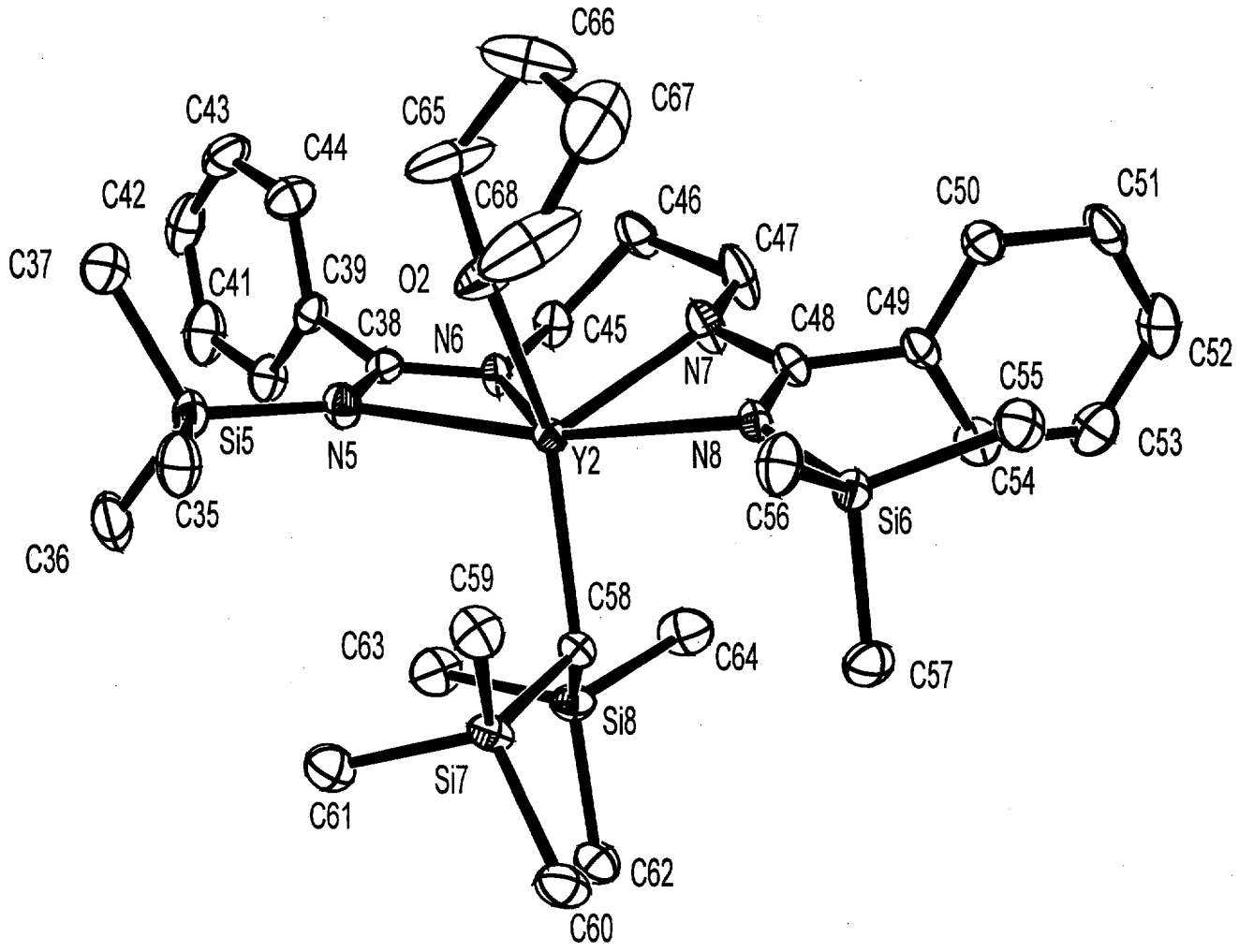
Y(2)	-O(2)	2.401(7)
Y(2)	-N(5)	2.461(7)
Y(2)	-N(6)	2.301(7)
Y(2)	-N(7)	2.284(8)
Y(2)	-N(8)	2.515(6)
Y(2)	-C(38)	2.781(7)
Y(2)	-C(48)	2.792(7)
Y(2)	-C(58)	2.436(8)
Si(5)	-N(5)	1.729(8)
Si(5)	-C(35)	1.873(10)
Si(5)	-C(36)	1.861(9)
Si(5)	-C(37)	1.864(10)
Si(6)	-N(8)	1.754(7)
Si(6)	-C(55)	1.854(8)
Si(6)	-C(56)	1.855(8)
Si(6)	-C(57)	1.843(8)
Si(7)	-C(58)	1.834(9)
N(5)	-C(38)	1.321(11)
N(6)	-C(38)	1.320(11)
N(6)	-C(45)	1.458(11)
N(7)	-C(47)	1.462(14)
N(7)	-C(48)	1.327(10)
N(8)	-C(48)	1.322(10)
C(38)	-C(39)	1.518(10)
C(39)	-C(40)	1.369(9)
C(39)	-C(44)	1.386(12)
C(40)	-C(41)	1.388(13)
C(41)	-C(42)	1.366(15)
C(42)	-C(43)	1.373(15)
C(43)	-C(44)	1.394(14)
C(45)	-C(46)	1.513(11)
C(46)	-C(47)	1.524(14)
C(48)	-C(49)	1.503(11)
C(49)	-C(50)	1.375(10)

Si(7)	-C(60)	1.867(8)	C(50)	-C(51)	1.402(13)
Si(7)	-C(61)	1.875(9)	C(51)	-C(52)	1.380(13)
Si(8)	-C(58)	1.827(9)	C(52)	-C(53)	1.394(13)
Si(8)	-C(62)	1.891(10)	C(53)	-C(54)	1.382(13)
Si(8)	-C(63)	1.872(8)	C(65)	-C(66)	1.490(17)
Si(8)	-C(64)	1.885(10)	C(66)	-C(67)	1.44(2)
O(2)	-C(65)	1.427(12)	C(67)	-C(68)	1.44(2)
O(2)	-C(68)	1.399(15)			

Bond Angles (deg.)

O(2)	-Y(2)	-N(5)	79.4(2)	C(62)	-Si(8)	-C(63)	105.7(4)
O(2)	-Y(2)	-N(6)	107.4(2)	C(62)	-Si(8)	-C(64)	106.2(5)
O(2)	-Y(2)	-N(7)	93.1(3)	C(63)	-Si(8)	-C(64)	107.3(5)
O(2)	-Y(2)	-N(8)	84.0(2)	Y(2)	-O(2)	-C(65)	118.1(7)
O(2)	-Y(2)	-C(38)	91.9(2)	Y(2)	-O(2)	-C(68)	129.7(6)
O(2)	-Y(2)	-C(48)	92.7(2)	C(65)	-O(2)	-C(68)	104.8(8)
O(2)	-Y(2)	-C(58)	145.2(3)	Y(2)	-N(5)	-Si(5)	143.9(4)
N(5)	-Y(2)	-N(6)	56.3(2)	Y(2)	-N(5)	-C(38)	89.4(5)
N(5)	-Y(2)	-N(7)	125.3(3)	Si(5)	-N(5)	-C(38)	126.6(6)
N(5)	-Y(2)	-N(8)	163.4(2)	Y(2)	-N(6)	-C(38)	96.6(5)
N(5)	-Y(2)	-C(38)	28.3(3)	Y(2)	-N(6)	-C(45)	136.1(5)
N(5)	-Y(2)	-C(48)	152.5(2)	C(38)	-N(6)	-C(45)	124.3(7)
N(5)	-Y(2)	-C(58)	102.1(3)	Y(2)	-N(7)	-C(47)	137.5(5)
N(6)	-Y(2)	-N(7)	75.6(2)	Y(2)	-N(7)	-C(48)	97.7(5)
N(6)	-Y(2)	-N(8)	130.8(2)	C(47)	-N(7)	-C(48)	119.8(8)
N(6)	-Y(2)	-C(38)	28.1(3)	Y(2)	-N(8)	-Si(6)	142.5(3)
N(6)	-Y(2)	-C(48)	102.5(2)	Y(2)	-N(8)	-C(48)	87.6(4)
N(6)	-Y(2)	-C(58)	101.7(3)	Si(6)	-N(8)	-C(48)	126.7(5)
N(7)	-Y(2)	-N(8)	55.7(2)	Y(2)	-C(38)	-N(5)	62.3(4)
N(7)	-Y(2)	-C(38)	99.7(3)	Y(2)	-C(38)	-N(6)	55.3(4)
N(7)	-Y(2)	-C(48)	28.1(2)	Y(2)	-C(38)	-C(39)	171.0(5)
N(7)	-Y(2)	-C(58)	112.5(3)	N(5)	-C(38)	-N(6)	117.1(7)
N(8)	-Y(2)	-C(38)	154.6(2)	N(5)	-C(38)	-C(39)	123.2(7)
N(8)	-Y(2)	-C(48)	28.2(2)	N(6)	-C(38)	-C(39)	119.7(8)
N(8)	-Y(2)	-C(58)	91.3(2)	C(38)	-C(39)	-C(40)	120.8(7)
C(38)	-Y(2)	-C(48)	127.8(2)	C(38)	-C(39)	-C(44)	120.4(6)
C(38)	-Y(2)	-C(58)	105.7(3)	C(40)	-C(39)	-C(44)	118.8(7)
C(48)	-Y(2)	-C(58)	99.3(3)	C(39)	-C(40)	-C(41)	121.5(9)
N(5)	-Si(5)	-C(35)	106.6(4)	C(40)	-C(41)	-C(42)	119.5(8)
N(5)	-Si(5)	-C(36)	111.9(4)	C(41)	-C(42)	-C(43)	120.1(9)
N(5)	-Si(5)	-C(37)	115.4(4)	C(42)	-C(43)	-C(44)	120.4(9)
C(35)	-Si(5)	-C(36)	110.5(4)	C(39)	-C(44)	-C(43)	119.7(8)
C(35)	-Si(5)	-C(37)	105.0(5)	N(6)	-C(45)	-C(46)	111.5(6)
C(36)	-Si(5)	-C(37)	107.2(5)	C(45)	-C(46)	-C(47)	115.4(8)
N(8)	-Si(6)	-C(55)	116.7(3)	N(7)	-C(47)	-C(46)	111.6(8)
N(8)	-Si(6)	-C(56)	109.4(4)	Y(2)	-C(48)	-N(7)	54.2(4)
N(8)	-Si(6)	-C(57)	110.7(4)	Y(2)	-C(48)	-N(8)	64.1(4)
C(55)	-Si(6)	-C(56)	104.0(4)	Y(2)	-C(48)	-C(49)	163.9(5)
C(55)	-Si(6)	-C(57)	106.5(4)	N(7)	-C(48)	-N(8)	116.4(7)
C(56)	-Si(6)	-C(57)	109.1(5)	N(7)	-C(48)	-C(49)	119.7(7)
C(58)	-Si(7)	-C(59)	109.5(4)	N(8)	-C(48)	-C(49)	124.0(6)
C(58)	-Si(7)	-C(60)	114.6(5)	C(48)	-C(49)	-C(50)	121.1(7)
C(58)	-Si(7)	-C(61)	113.5(4)	C(48)	-C(49)	-C(54)	118.9(7)
C(59)	-Si(7)	-C(60)	105.5(4)	C(50)	-C(49)	-C(54)	120.0(8)

C(60)	-Si(7)	-C(61)	106.7(4)	C(50)	-C(51)	-C(52)	119.2(8)
C(58)	-Si(8)	-C(62)	114.3(4)	C(51)	-C(52)	-C(53)	119.9(8)
C(58)	-Si(8)	-C(63)	112.9(4)	C(52)	-C(53)	-C(54)	120.5(9)
C(58)	-Si(8)	-C(64)	110.0(4)	C(49)	-C(54)	-C(53)	119.8(8)
Y(2)	-C(58)	-Si(7)	105.4(4)	C(65)	-C(66)	-C(67)	105.0(12)
Y(2)	-C(58)	-Si(8)	121.0(4)	C(66)	-C(67)	-C(68)	105.7(11)
Si(7)	-C(58)	-Si(8)	119.2(5)	O(2)	-C(68)	-C(67)	105.3(11)
O(2)	-C(65)	-C(66)	105.9(9)				



17

Molecule 2